Unraveling the effectual binding potential of carbon nanotubes and norfullerene against multiple targets of SARS-CoV-2 by computational modeling and virtual screening

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Abstract

COVID-19 became a potential healthcare concern and the latest variants of SARS CoV-2 resulted in massive transmission of the diseases. Though several vaccines are available, no potential drug candidates developed yet. Thus, the present study aimed to predict the possibility of carbon-based nanoparticles as the probable drug candidates towards the selected targets of SARS-CoV-2. The 3D structures of carbon-based nanoparticles such as nanotubes and nano-fullerene were predicted computationally, and the effectual binding of these nanoparticles to spike glycoprotein, main protease, papain-like protease, and RNA binding domain of the nucleocapsid proteins of SARS-CoV-2 was also predicted by molecular docking. The interaction stability of the best-docked complex was further validated by molecular dynamic (MD) simulations. The pharmacophoric features and ADMET properties of the carbon nanomaterials were predicted. This study revealed that carbon fullerene and nanotube showed potential effectual binding with the prioritized multi-targets of SARS-CoV-2. The study further depicted that carbon nanotube showed better effectual binding to the selected targets than carbon fullerene. The dynamic simulation studies revealed that the binding of nanoparticles

with selected targets was stable throughout the interaction trajectories. Thus, the present study illustrated that carbon nanotubes and fullerene can be effective binders against several targets of SARS-CoV-2, and the study can be scaled up in experimental level to validate the hypothesis and design novel nanomaterial-based drug formulations against SARS-CoV-2.

Keywords: COVID-19, SARS-CoV-2, Multiple targets, Carbon nanotubes, Carbon norfullerene, Effectual binding